

FIGURE 1

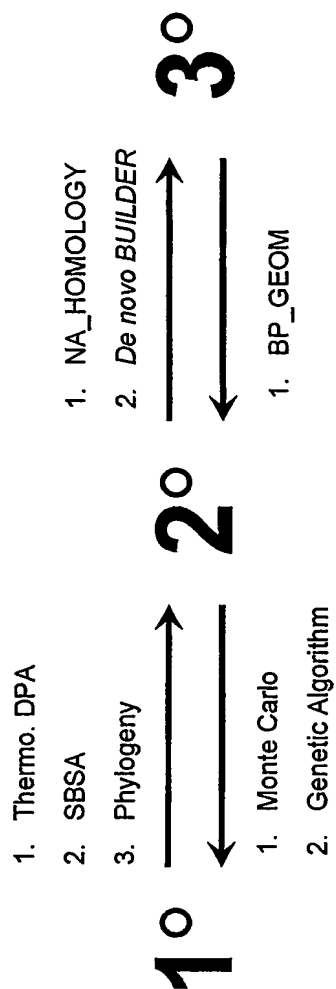




FIGURE 3

**Homology Modeling**

**Input File Window**

C:\Documents and Settings\John SantaLucia\Desktop\SS project 5-1-04\1JJ2\_5S  
added bases 5-25-04 2.PDB **BROWSE...**

**Load information from input file** 122 residues were found in input file

**Alignment window**

UUAGGCGGCCACAGCGGUGGGGUUGCCUCCCGUACCCAUCCCGAACACGGAAGAUAGCCACC  
vvvvv COPY BELOW vvvvvv

**Load new sequence from the file** **SBSA** **Update Substitution List**

**Substitution Window -- (All Data is CASE Sensitive)**

Residues from input for: Chain: 9

Residue	Chain
U	1
U	2
A	3
G	4
G	5
C	6
G	7
G	8
C	9
C	10
A	11

122 residues were found for this chain! **Load from a file ...**

**Options**

- ☒ Add hydrogens
- ☐ Print initial energy
- ☐ Print final energy
- ☐ Close deletion gaps
- ☐ Close insertion gaps
- ☐ Optimize with Powell
- ☐ DSTA on substituted
- ☒ DSTA on all residues
- ☐ DSTA on positive ends
- ☐ Leave only R atoms
- ☐ Remove Bases

**UPDATE LIST** **Delete selected**

**Only for testing:**  
Counter 0  
Gap Size (RMSD) 0

**Compute, Print H-bonds** **RMSD**

**Message Window**

Performing Chi Dihedral optimization for missing bases... Done!

**Output File Window**

C:\Documents and Settings\John SantaLucia\Desktop\SS project 5-1-04\1JJ2\_5S  
added bases 5-25-04 2.PDB **BROWSE...**

**Save data in output file** **END PROGRAM**

FIGURE 4

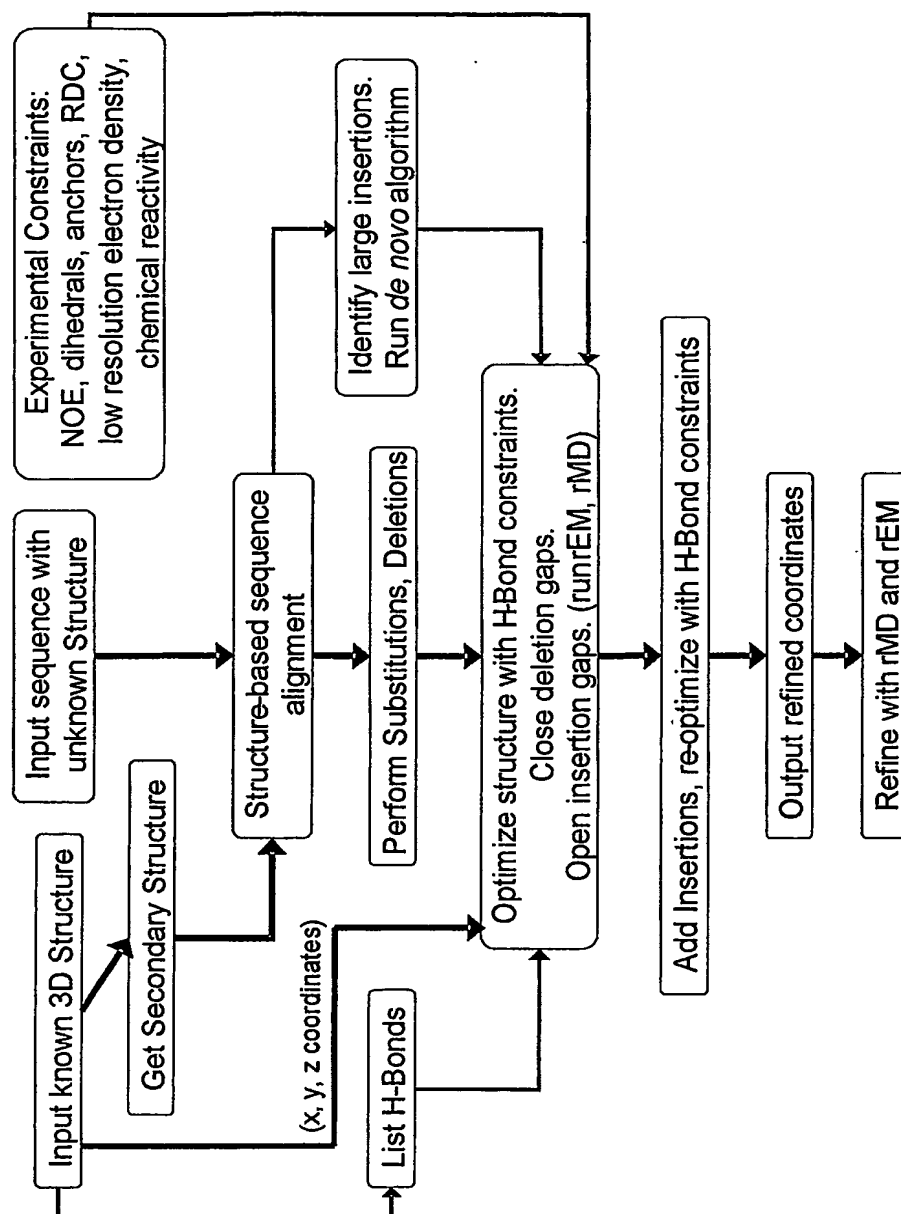


FIGURE 5

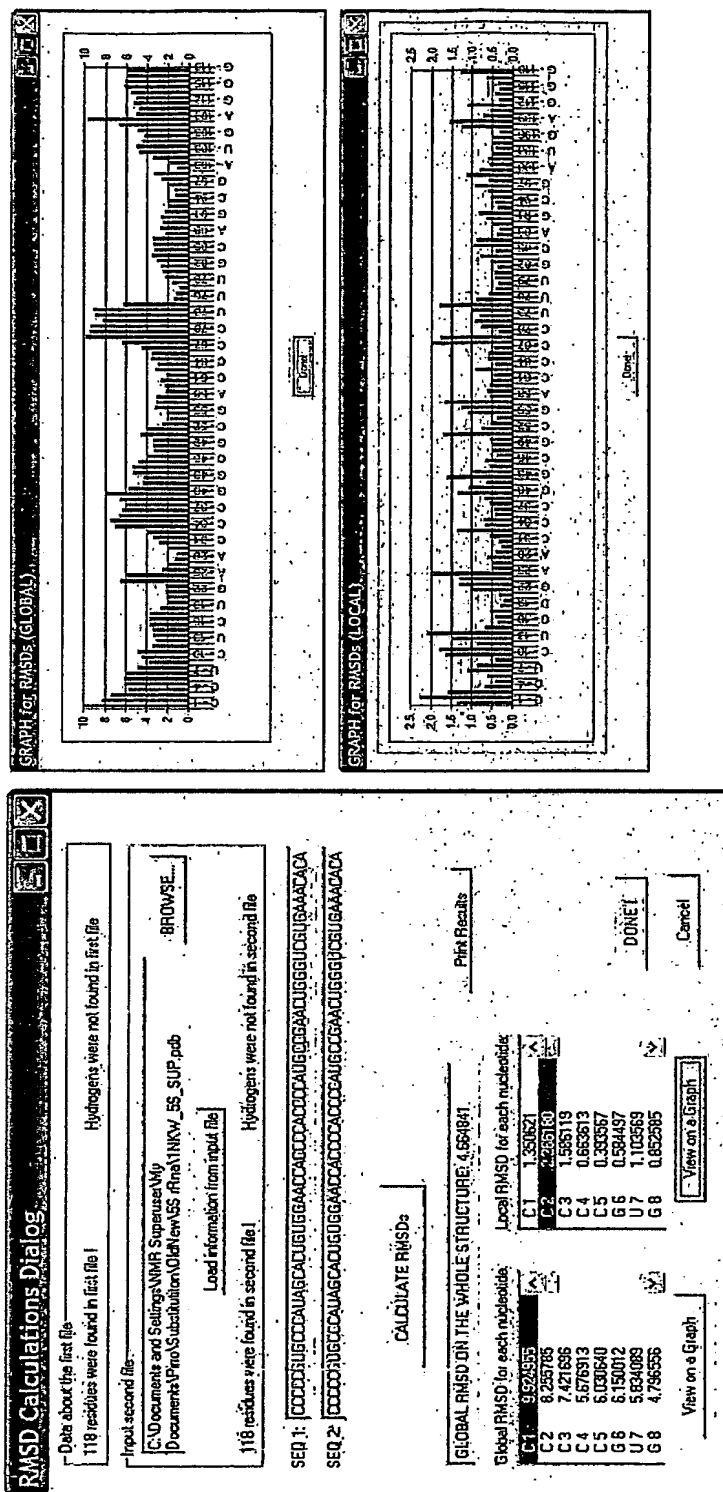


FIGURE 6

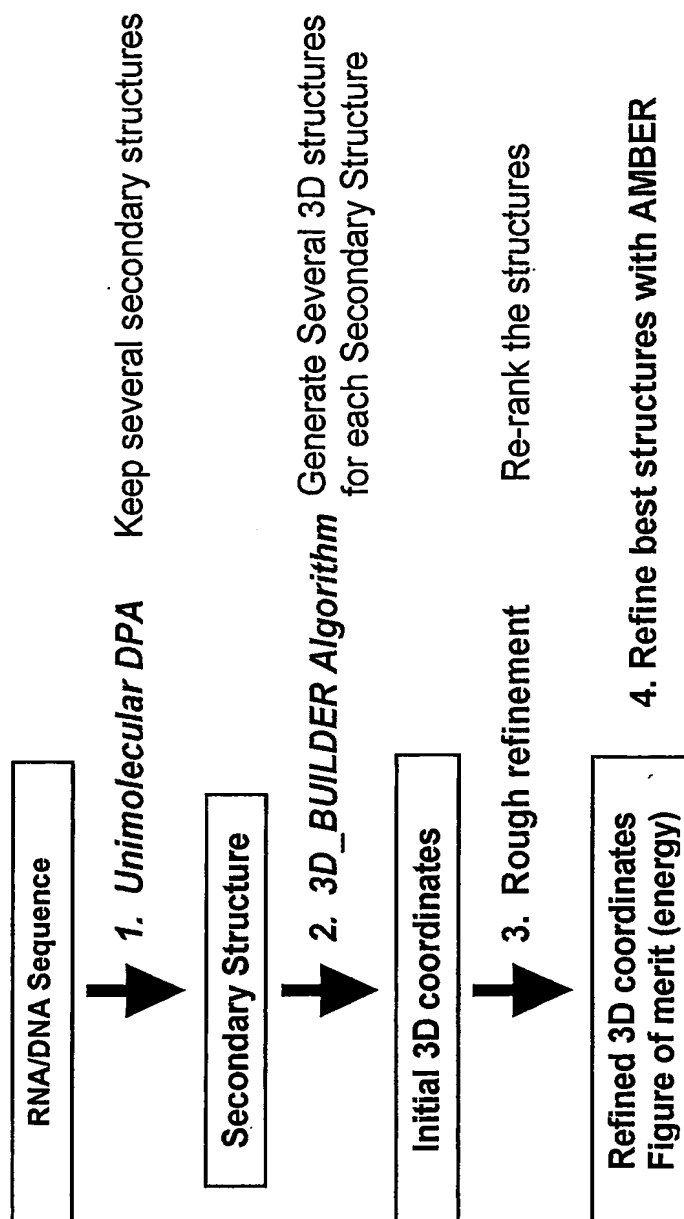


FIGURE 7

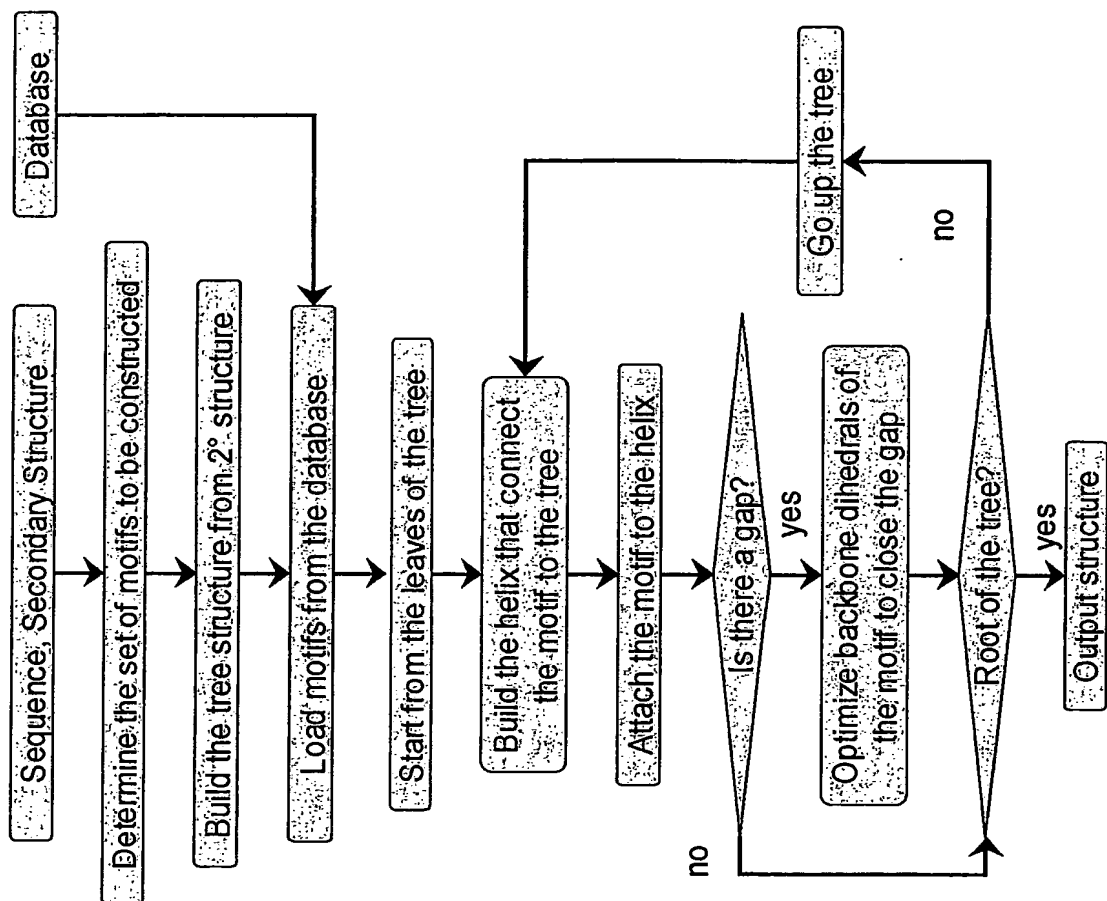


FIGURE 8

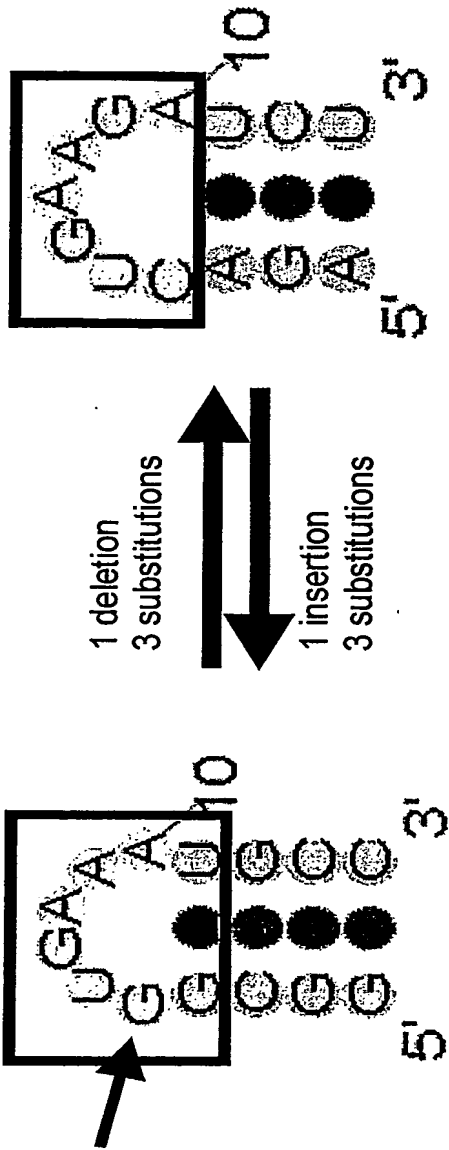




FIGURE 9

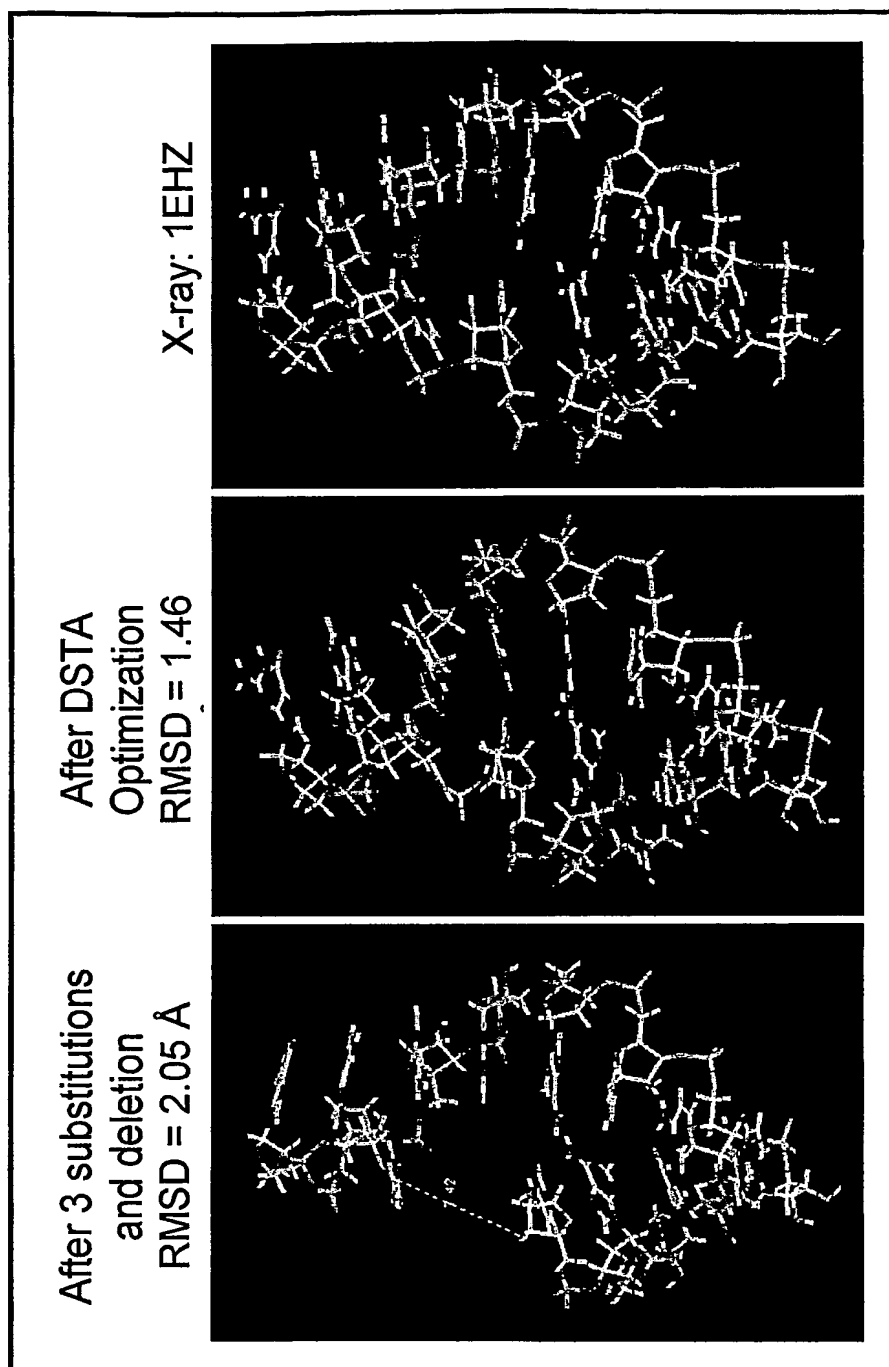
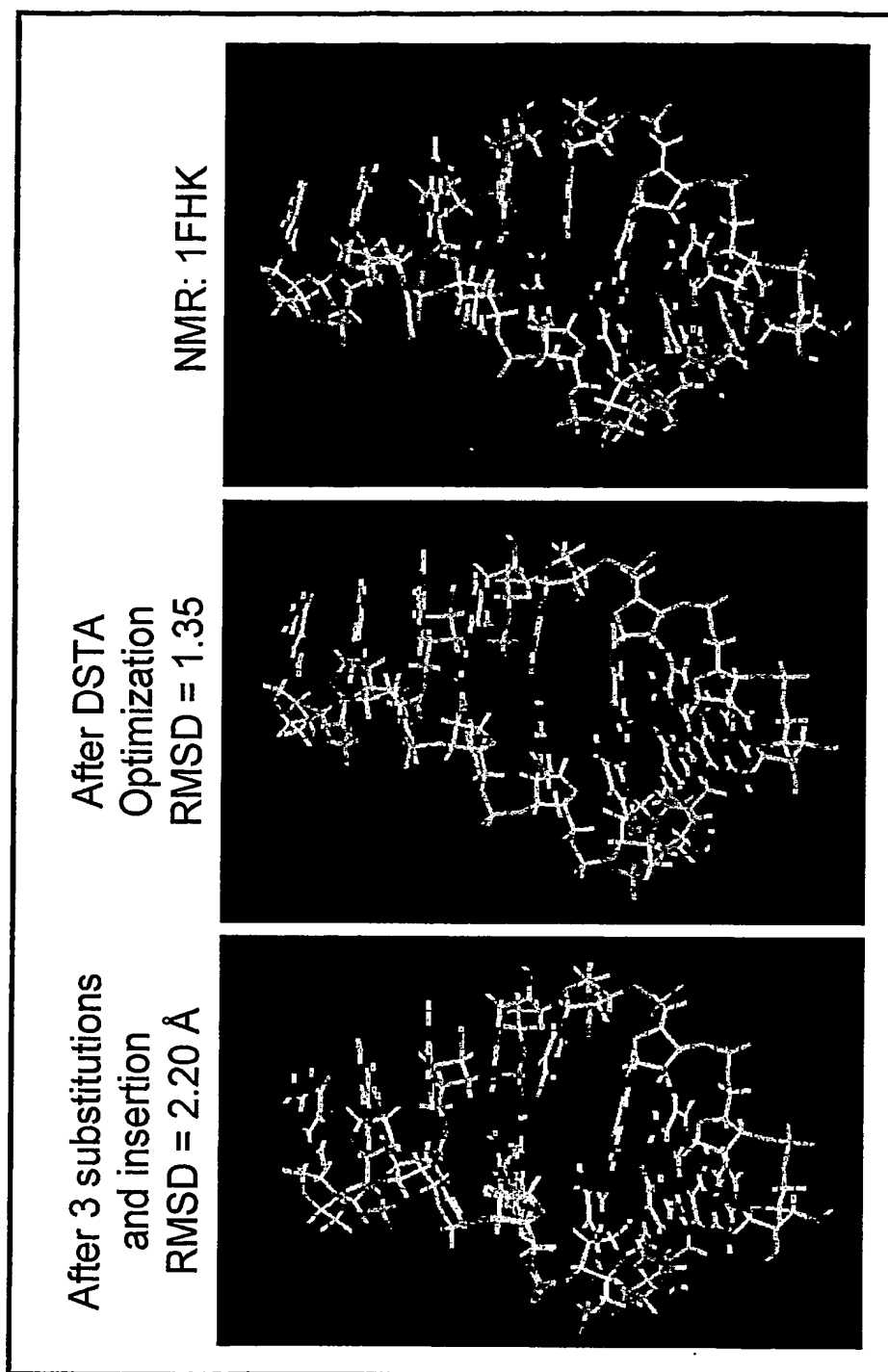


FIGURE 10



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## FIGURE 11

Motif type: Hairpin  
 Motif size: 3  
 Sequences: CUCAG, CUAAG  
 Source: 1NKW  
 Positions 331-333  
 Resolution: 3.0  

ATOM 6145	P	C	O	330	-42.207	137.234	85.023	1.00	48.85	P
ATOM 6146	O1P	C	O	330	-43.221	138.159	84.459	1.00	48.85	O
ATOM 6147	O2P	C	O	330	-41.551	136.236	84.137	1.00	48.85	O
ATOM 6148	O5*	C	O	330	-41.069	138.098	85.722	1.00	48.85	O
ATOM 6149	C5*	C	O	330	-41.357	138.842	86.901	1.00	48.85	C
ATOM 6150	C4*	C	O	330	-40.085	139.347	87.534	1.00	48.85	C
ATOM 6151	O4*	C	O	330	-39.275	138.237	88.009	1.00	48.85	O
ATOM 6152	C3*	C	O	330	-39.142	140.097	86.615	1.00	48.85	C
ATOM 6153	O3*	C	O	330	-39.580	141.430	86.387	1.00	48.85	O
ATOM 6154	C2*	C	O	330	-37.842	140.026	87.402	1.00	48.85	C
ATOM 6155	O2*	C	O	330	-37.815	140.934	88.486	1.00	48.85	O
ATOM 6156	C1*	C	O	330	-37.898	138.592	87.935	1.00	48.85	C

 Chi DIHEDRAL = -3.10169 radians  
 C4'-O4'-C1'-N9 DIHEDRAL = -2.11876 radians  
 O4'-C1'-N9 bond angle = 1.90932 radians

FIGURE 12

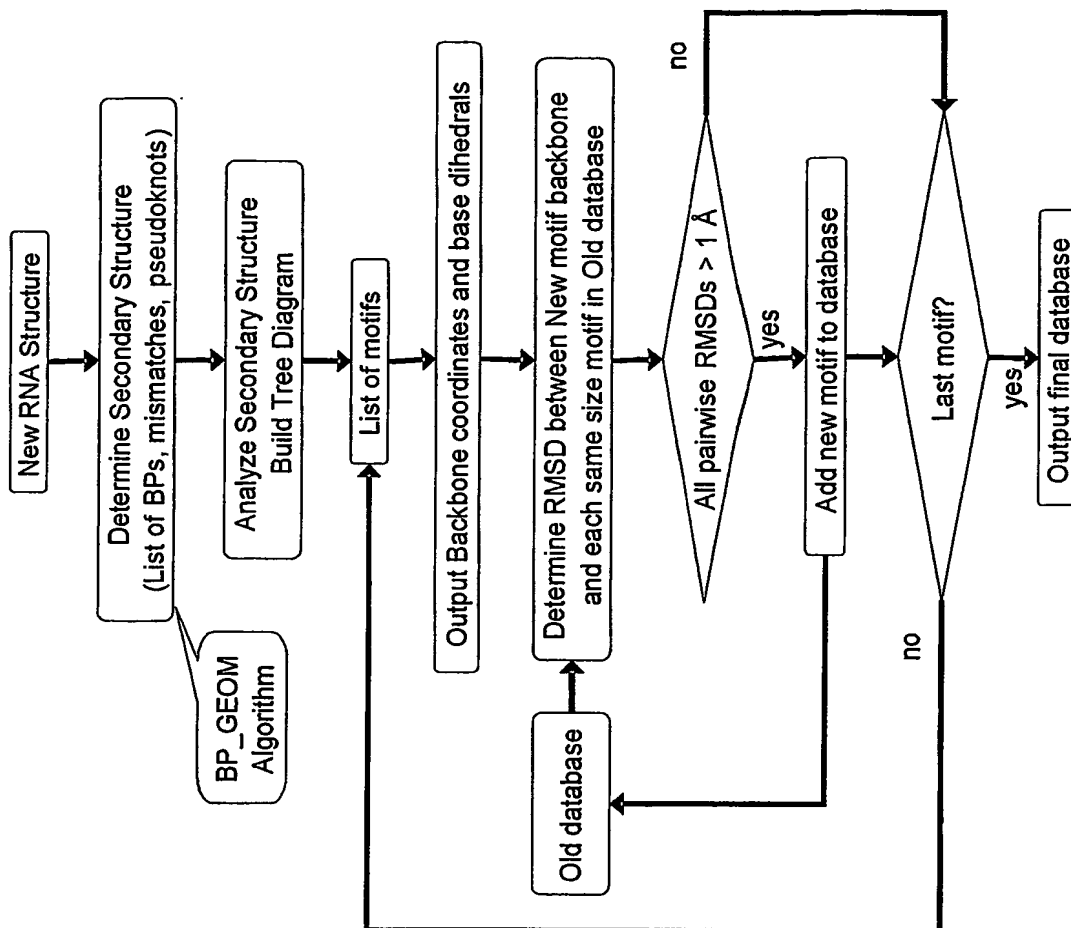


FIGURE 13

Hairpins <sup>a,b,c,d,e</sup>	Bulges <sup>b,c,d,e</sup>	Internal Loops <sup>b,c,d,e</sup>	Multiloops
Length    Number	Length    Number	Length    Number	stems         Number
3              6	1              31	1x1          42	3x9          1 3              55
4              64	2              15	1x2          18	4x4          6 4              28
5              23	3              1	1x3          12	4x5          15 5              11
6              20	4              0	1x4          8	4x6          3 6              4
7              26	5              0	1x5          1	4x7          3 7              2
8              23	6              2	2x2          13	5x5          6 11             1
9              16	7              0	2x3          15	5x6          12
10             11	8              0	2x4          7	5x7          7
11             8	9              1	2x5          2	5x8          5
12             6		2x6          2	6x6          4
13             4		2x7          1	6x7          4
14             0		3x3          17	7x7          3
15             5		3x4          11	other        24
19             1		3x5          5	
		3x6          4	
		3x7          5	
<b>References for crystal structures</b>			
a 1EHZ tRNAphe			
b 1HR2 group I intron			
c 1J5E 16S rRNA <i>Thermus thermophilus</i>			
d 1JJ2 23S rRNA <i>Haloarcula marismortui</i>			
e 1NKW 23S rRNA <i>Deinococcus Radiodurans</i>			

## FIGURE 14

CLUSTAL-W sequence alignment of 5S rRNA

Score = 68/129 = 52.7%

Correct alignment = 100/129 = 77.5%

```

1JJ2  ---UUAGGCGGCCACAGCGGUGGGUUGCCUCCGUACCCAUCCGGAACACGGAAGUAAG
1NKW  ACACCCCGUGCCCAUAGCACUGUGGA-ACCACCCACCCCAUGCCGAACUGGGUCGUGAAA
      * * *** ** ** ** * * *** **** * * * *

```

```

1JJ2  CCCACCAGCGUUCGGGGAGUACUGGAGUGCGGAGCCUCUGGGAACCCGGUU--CGCCGCCACC-
1NKW  CACAGCAGCG--CCAAUGA-UACUCGGAC-CGCAGGGUCCCGGAAAGUCGGUCAGCGCGGGGUUU
      * * ***** ** ** ***** * * * * * * * * * *

```

SBSA Alignment of 5S rRNA

IDENT = 65/129 = 50.4%

Correct alignment = 129/129 = 100%

```

1JJ2  ddd LLLLLL d LLLLLLLL i mLLLLLLL RRRR RRm
1NKW  ---UUAGGCGGCC-ACAGCGGUGGGUUGCCUCCGUACCCAUCCGGAACACGGAAGUAAG
      ACACCCCGUGCCCAUAGCACUGUGGA-ACCACCCACCCCAUGCCGAACUGGGUCGUGAAA
      LLLLLLLLLL i LmLLLLL d LLLLLLL RRRR RRR
      -- *** *-***- ** ** -** *** ***** ** * *-
1JJ2  RRRRRR RR mLLLLL i LLLLLLlL RRRRRRR RRRRmm RRRRR ddd
1NKW  CCCACCAGCGUUCGGGGAGUACUGGAGUGCGGAGCCUCUGGGAACCCGGUUCGCCGCCACC-
      CACAGCAGCG--CCAAUGA-UACUCGGA-CCGAGGGUCCCGGAAAGUCGGUCAGCGCGGGGUUU
      RRRRRm RR ddLmLL d LmLLLLdLl RRRRRmRR RRmRR RRRRRRRRRi
      * * ***** **-- ** ***** *-- ***--* -***-*** -***- **

```

FIGURE 15

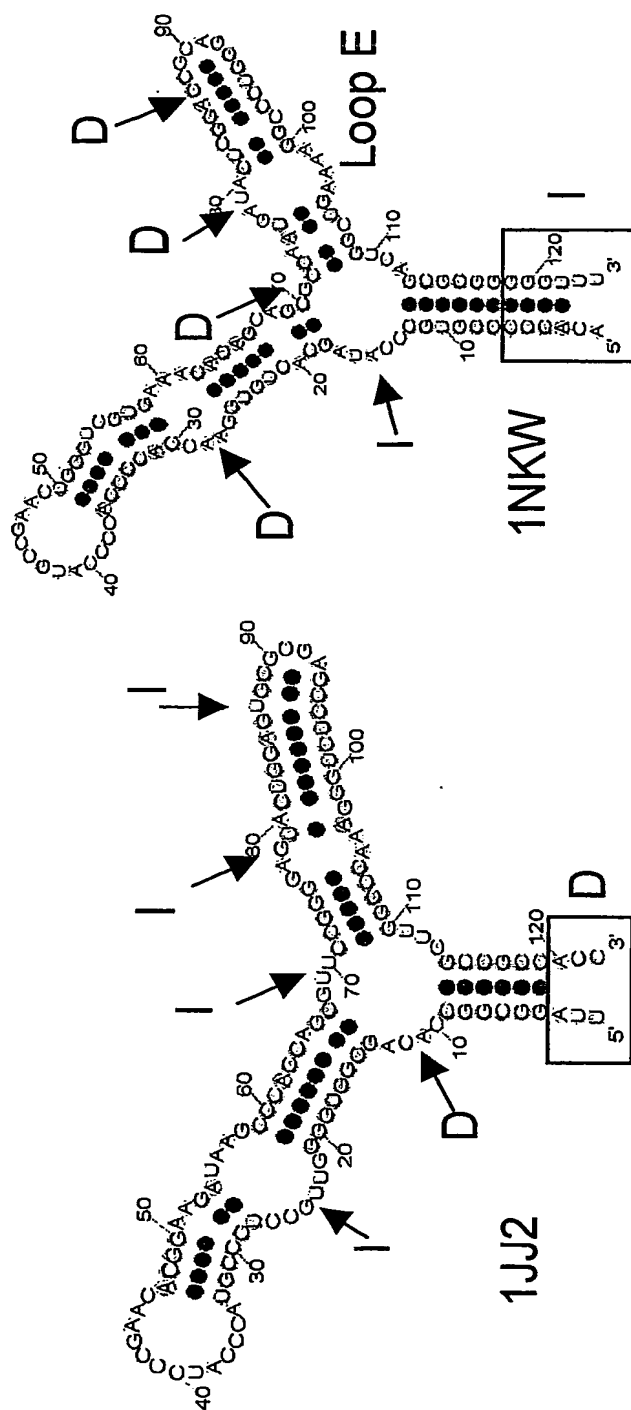


FIGURE 16

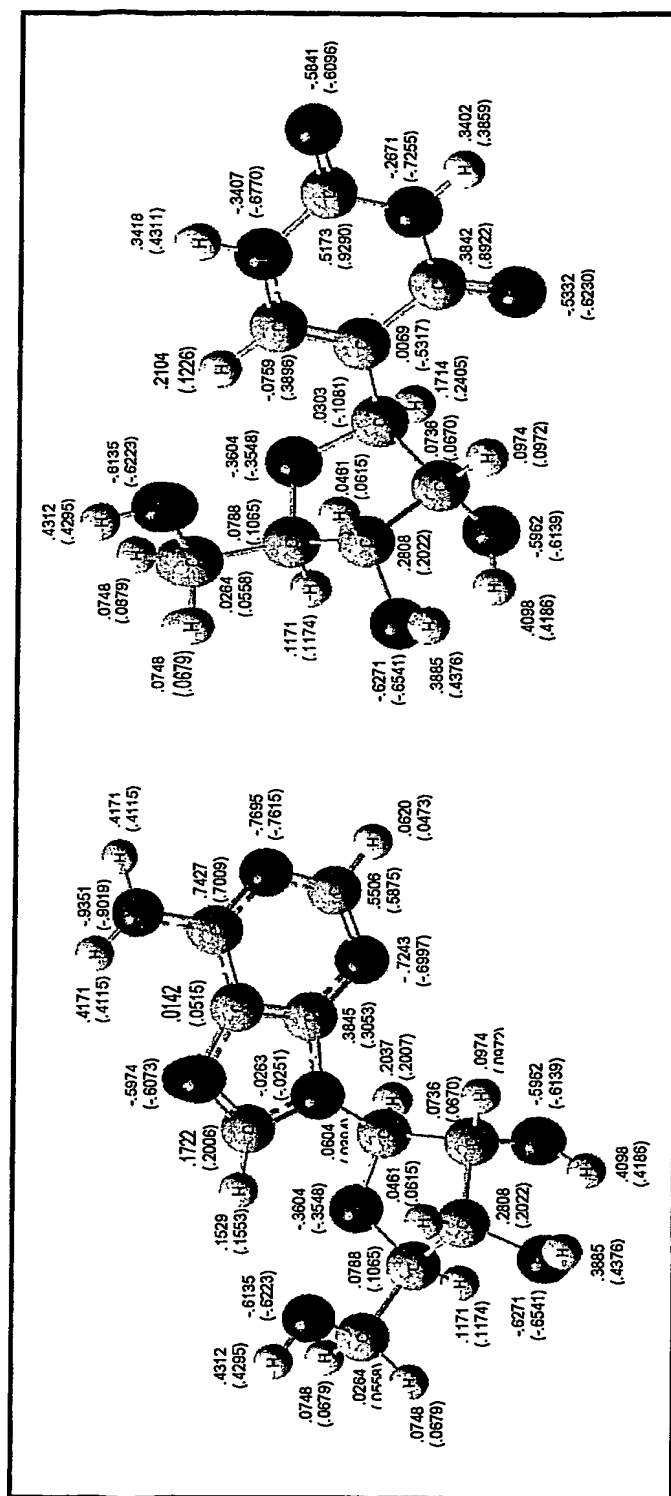




FIGURE 17

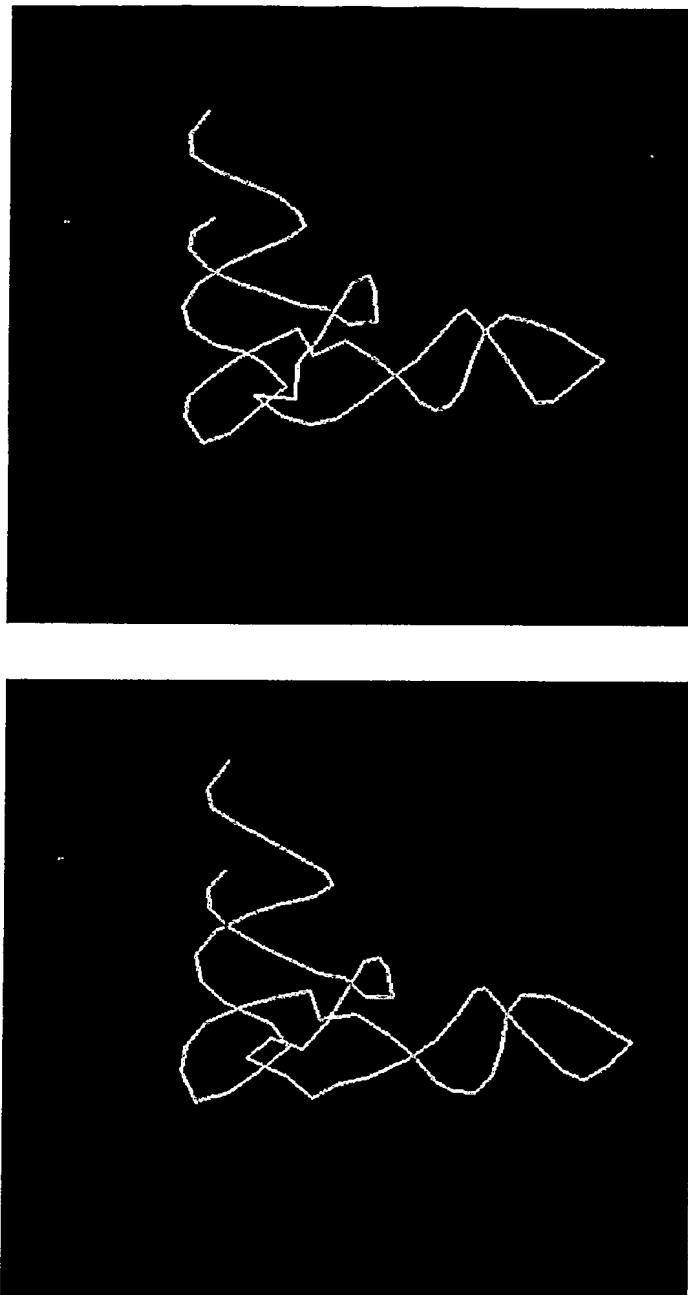


FIGURE 18

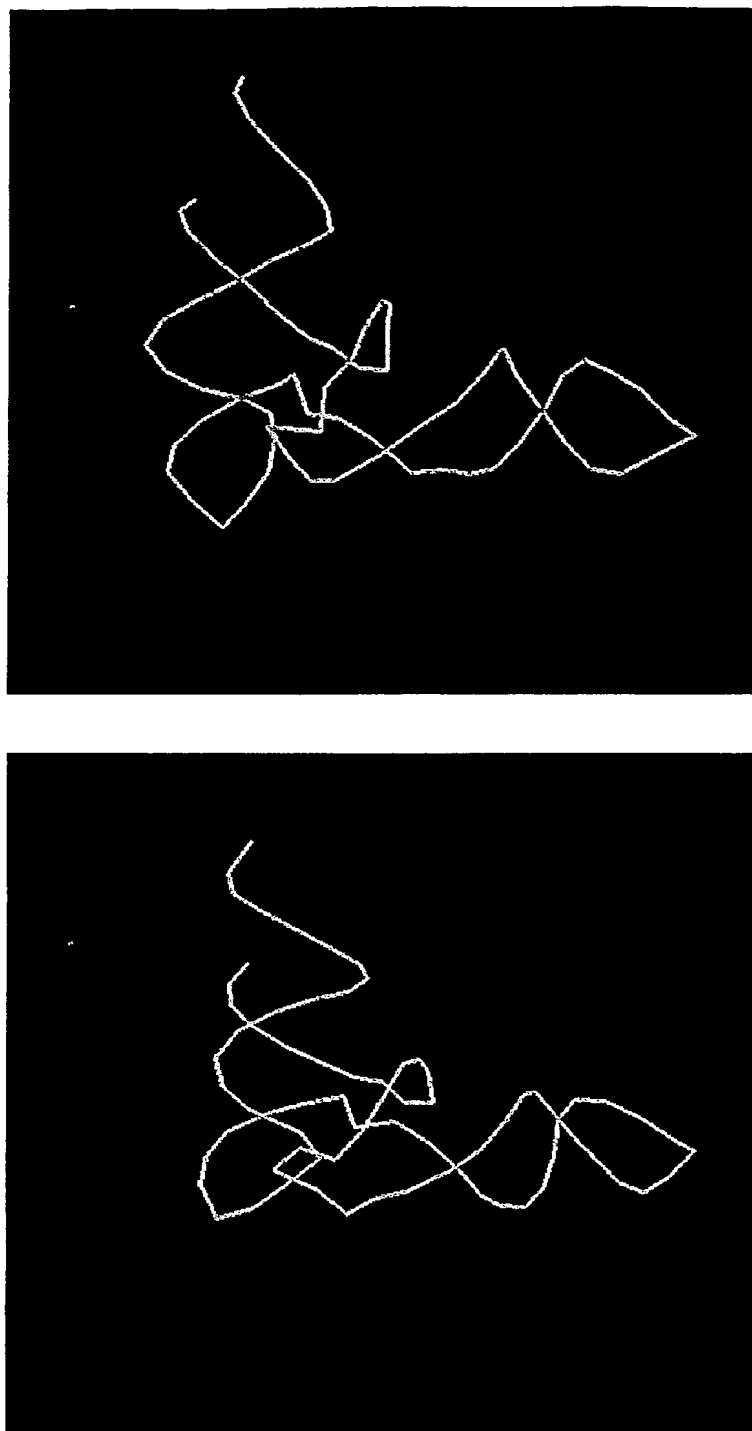


FIGURE 19

